Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 09:59 PM EDT

PDB ID	:	2CYP
Title	:	Crystal structure of yeast cytochrome C peroxidase refined at 1.7-angstroms resolution
Authors	:	Finzel, B.C.; Poulos, T.L.; Kraut, J.
Deposited on	:	1985-08-27
Resolution	:	1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

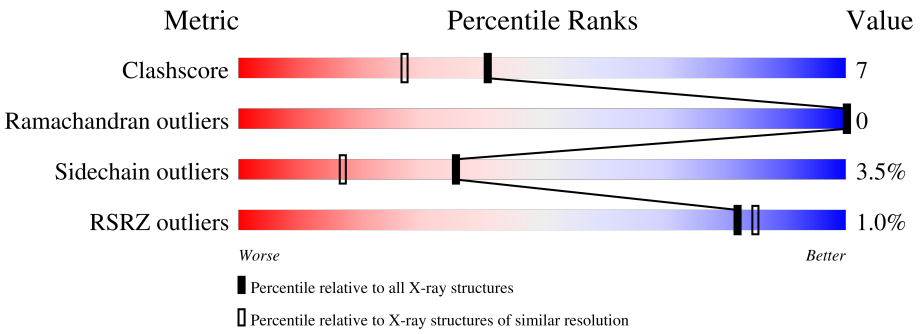
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	294	% 66% 29% 5%

2 Entry composition (i)

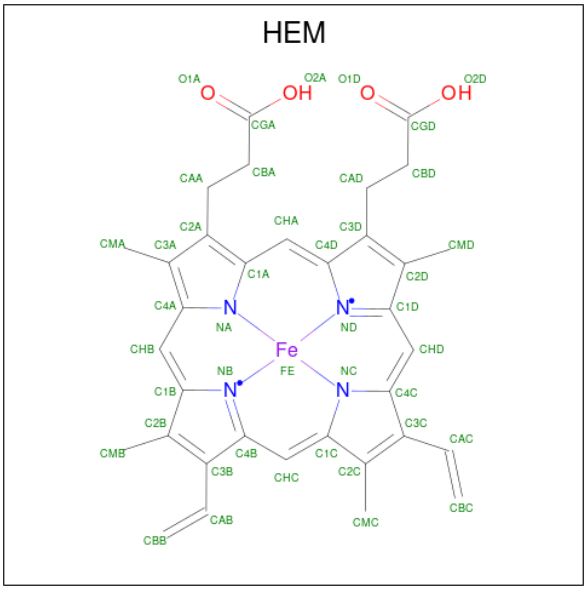
There are 4 unique types of molecules in this entry. The entry contains 2609 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CYTOCHROME C PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	293	2303	1477	378	442	6	0	2	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0

- Molecule 3 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	1	1	1	0	0

- Molecule 4 is water.

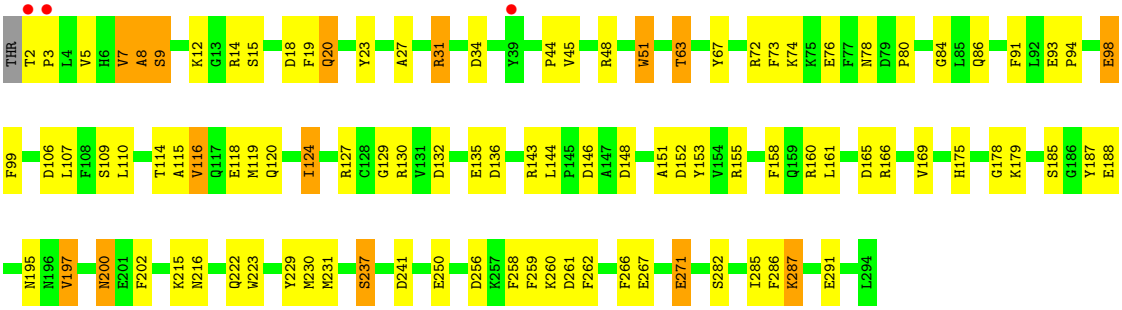
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	262	262	262	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CYTOCHROME C PEROXIDASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.40Å 76.80Å 51.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.70 15.21 – 1.66	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.70) 87.4 (15.21-1.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.20 (at 1.66Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.202 , (Not available) 0.183 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 69.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2609	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, O

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.20	3/2381 (0.1%)	2.19	113/3237 (3.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	187	TYR	CG-CD1	6.19	1.47	1.39
1	A	262	PHE	CG-CD2	5.31	1.46	1.38
1	A	259	PHE	N-CA	5.26	1.56	1.46

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	48	ARG	NE-CZ-NH1	18.64	129.62	120.30
1	A	14	ARG	NE-CZ-NH2	-16.20	112.20	120.30
1	A	166	ARG	NE-CZ-NH2	-16.14	112.23	120.30
1	A	72	ARG	NE-CZ-NH2	14.76	127.68	120.30
1	A	165	ASP	CB-CG-OD1	11.64	128.77	118.30
1	A	258	PHE	CB-CG-CD2	-11.18	112.98	120.80
1	A	261	ASP	CB-CG-OD1	10.91	128.12	118.30
1	A	202	PHE	CB-CG-CD2	-10.70	113.31	120.80
1	A	229	TYR	CB-CG-CD1	-10.67	114.60	121.00
1	A	31	ARG	NE-CZ-NH2	-10.58	115.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	106	ASP	CB-CG-OD1	10.53	127.78	118.30
1	A	48	ARG	NE-CZ-NH2	-10.48	115.06	120.30
1	A	258	PHE	CB-CG-CD1	10.30	128.01	120.80
1	A	285	ILE	CB-CG1-CD1	10.00	141.90	113.90
1	A	260	LYS	CA-CB-CG	9.58	134.47	113.40
1	A	34	ASP	CB-CG-OD2	-9.49	109.76	118.30
1	A	132	ASP	CB-CG-OD1	9.44	126.80	118.30
1	A	262	PHE	CB-CG-CD1	9.14	127.20	120.80
1	A	34	ASP	CB-CG-OD1	8.99	126.39	118.30
1	A	118	GLU	OE1-CD-OE2	-8.83	112.70	123.30
1	A	215	LYS	CA-CB-CG	8.79	132.73	113.40
1	A	241	ASP	CB-CG-OD1	8.65	126.09	118.30
1	A	197	VAL	CG1-CB-CG2	8.56	124.60	110.90
1	A	229	TYR	CB-CG-CD2	8.51	126.11	121.00
1	A	130	ARG	NE-CZ-NH2	8.48	124.54	120.30
1	A	107	LEU	O-C-N	8.12	135.69	122.70
1	A	152	ASP	CB-CG-OD1	8.09	125.58	118.30
1	A	187	TYR	CB-CG-CD1	-8.04	116.17	121.00
1	A	18	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	A	31	ARG	NH1-CZ-NH2	7.89	128.08	119.40
1	A	14	ARG	NH1-CZ-NH2	7.79	127.97	119.40
1	A	187	TYR	CG-CD1-CE1	-7.75	115.10	121.30
1	A	160	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	A	91	PHE	CB-CG-CD1	-7.70	115.41	120.80
1	A	63[A]	THR	CA-CB-CG2	7.65	123.11	112.40
1	A	63[B]	THR	CA-CB-CG2	7.65	123.11	112.40
1	A	262	PHE	CB-CG-CD2	-7.55	115.51	120.80
1	A	166	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	A	148	ASP	CB-CG-OD1	7.46	125.01	118.30
1	A	44	PRO	O-C-N	-7.38	110.89	122.70
1	A	7	VAL	CB-CA-C	7.36	125.39	111.40
1	A	262	PHE	O-C-N	7.34	134.45	122.70
1	A	291	GLU	OE1-CD-OE2	-7.21	114.65	123.30
1	A	9	SER	N-CA-CB	7.19	121.28	110.50
1	A	72	ARG	NH1-CZ-NH2	-7.16	111.52	119.40
1	A	130	ARG	NH1-CZ-NH2	-7.13	111.56	119.40
1	A	146	ASP	CB-CG-OD2	-7.11	111.91	118.30
1	A	31	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	A	130	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	266	PHE	CB-CG-CD1	-6.95	115.94	120.80
1	A	258	PHE	O-C-N	6.87	133.69	122.70
1	A	31	ARG	N-CA-CB	6.79	122.83	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	266	PHE	O-C-N	6.78	133.55	122.70
1	A	260	LYS	CB-CA-C	6.70	123.79	110.40
1	A	12	LYS	CA-C-O	6.61	133.98	120.10
1	A	45	VAL	CA-CB-CG1	6.51	120.66	110.90
1	A	266	PHE	CB-CG-CD2	6.50	125.35	120.80
1	A	158	PHE	CB-CG-CD1	-6.49	116.26	120.80
1	A	19	PHE	CB-CG-CD1	-6.49	116.26	120.80
1	A	197	VAL	CA-CB-CG2	6.37	120.46	110.90
1	A	116	VAL	CG1-CB-CG2	6.14	120.73	110.90
1	A	169	VAL	O-C-N	6.13	132.50	122.70
1	A	98	GLU	OE1-CD-OE2	6.03	130.53	123.30
1	A	175	HIS	N-CA-CB	6.02	121.43	110.60
1	A	31	ARG	CB-CA-C	-5.99	98.43	110.40
1	A	91	PHE	CB-CG-CD2	5.87	124.91	120.80
1	A	135	GLU	CA-CB-CG	5.86	126.29	113.40
1	A	109	SER	CB-CA-C	5.82	121.15	110.10
1	A	153	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	A	144	LEU	CB-CG-CD1	-5.74	101.24	111.00
1	A	27	ALA	N-CA-CB	5.73	118.12	110.10
1	A	178	GLY	O-C-N	5.73	131.86	122.70
1	A	73	PHE	CB-CG-CD1	5.69	124.78	120.80
1	A	73	PHE	CB-CG-CD2	-5.68	116.82	120.80
1	A	51	TRP	CB-CA-C	5.68	121.76	110.40
1	A	136	ASP	CB-CG-OD1	5.67	123.41	118.30
1	A	67	TYR	CB-CG-CD1	-5.65	117.61	121.00
1	A	187	TYR	CB-CG-CD2	5.63	124.38	121.00
1	A	185	SER	O-C-N	5.60	132.72	123.20
1	A	153	TYR	CB-CG-CD1	5.58	124.35	121.00
1	A	20	GLN	N-CA-CB	5.50	120.50	110.60
1	A	256	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	250	GLU	CG-CD-OE2	-5.44	107.42	118.30
1	A	7	VAL	CG1-CB-CG2	5.40	119.55	110.90
1	A	114	THR	O-C-N	5.38	131.30	122.70
1	A	130	ARG	O-C-N	5.37	131.29	122.70
1	A	124	ILE	O-C-N	5.35	131.26	121.10
1	A	63[A]	THR	OG1-CB-CG2	5.33	122.26	110.00
1	A	63[B]	THR	OG1-CB-CG2	5.33	122.26	110.00
1	A	237	SER	CB-CA-C	5.30	120.18	110.10
1	A	161[A]	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	161[B]	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	144	LEU	CB-CG-CD2	-5.24	102.09	111.00
1	A	271	GLU	CG-CD-OE1	5.23	128.77	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	118	GLU	N-CA-CB	5.23	120.02	110.60
1	A	14	ARG	CD-NE-CZ	-5.23	116.28	123.60
1	A	179	LYS	CA-CB-CG	5.22	124.88	113.40
1	A	31	ARG	CG-CD-NE	-5.21	100.86	111.80
1	A	187	TYR	N-CA-CB	5.21	119.97	110.60
1	A	119	MET	CG-SD-CE	5.19	108.51	100.20
1	A	231	MET	N-CA-CB	5.18	119.93	110.60
1	A	286	PHE	CB-CG-CD2	5.15	124.41	120.80
1	A	8	ALA	N-CA-CB	-5.13	102.92	110.10
1	A	110	LEU	CB-CG-CD1	5.09	119.66	111.00
1	A	151	ALA	CB-CA-C	5.09	117.73	110.10
1	A	260	LYS	CG-CD-CE	5.07	127.10	111.90
1	A	250	GLU	CA-C-O	-5.05	109.49	120.10
1	A	155	ARG	N-CA-CB	5.04	119.66	110.60
1	A	5	VAL	CB-CA-C	5.03	120.95	111.40
1	A	115	ALA	CB-CA-C	5.02	117.63	110.10
1	A	120	GLN	C-N-CA	5.01	132.82	122.30
1	A	282	SER	N-CA-CB	-5.01	102.99	110.50
1	A	18	ASP	OD1-CG-OD2	5.00	132.81	123.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	63[A]	THR	CB
1	A	63[B]	THR	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	ARG	Sidechain
1	A	31	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2303	0	2096	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	43	0	30	0	0
3	A	1	0	0	0	0
4	A	262	0	0	2	0
All	All	2609	0	2126	32	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (32) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLY:H	1:A:86:GLN:HE22	1.16	0.92
1:A:84:GLY:N	1:A:86:GLN:HE22	1.75	0.85
1:A:63[A]:THR:CG2	1:A:143:ARG:HH12	1.94	0.81
1:A:20:GLN:HE22	1:A:287:LYS:H	1.30	0.76
1:A:98:GLU:HG2	1:A:99:PHE:CE1	2.23	0.73
1:A:63[A]:THR:HG21	1:A:143:ARG:HH12	1.53	0.72
1:A:216:ASN:HD22	1:A:222:GLN:HE21	1.37	0.71
1:A:216:ASN:HD22	1:A:222:GLN:NE2	1.90	0.70
1:A:63[A]:THR:CG2	1:A:143:ARG:HH22	2.08	0.65
1:A:200:ASN:H	1:A:200:ASN:HD22	1.50	0.59
1:A:63[A]:THR:HG23	1:A:143:ARG:HH22	1.66	0.59
1:A:98:GLU:HG2	1:A:99:PHE:CD1	2.37	0.59
1:A:188:GLU:H	1:A:222:GLN:HE22	1.52	0.56
1:A:116:VAL:HG11	1:A:124:ILE:HD11	1.89	0.54
1:A:76:GLU:HB2	4:A:676:HOH:O	2.06	0.54
1:A:63[A]:THR:HG23	1:A:143:ARG:NH2	2.21	0.54
1:A:63[A]:THR:CG2	1:A:143:ARG:NH1	2.68	0.52
1:A:84:GLY:H	1:A:86:GLN:NE2	1.96	0.50
1:A:2:THR:N	1:A:3:PRO:HD3	2.27	0.50
1:A:267:GLU:OE1	1:A:271:GLU:OE1	2.31	0.49
1:A:195:ASN:HD22	1:A:195:ASN:H	1.60	0.49
1:A:63[A]:THR:HG22	1:A:143:ARG:HH22	1.78	0.48
1:A:86:GLN:NE2	1:A:86:GLN:H	2.12	0.47
1:A:8:ALA:HA	1:A:129:GLY:O	2.15	0.47
1:A:84:GLY:N	1:A:86:GLN:NE2	2.54	0.46
1:A:74:LYS:O	1:A:78:ASN:HB2	2.17	0.45
1:A:84:GLY:CA	1:A:86:GLN:NE2	2.81	0.44
1:A:15:SER:HB2	4:A:316:HOH:O	2.19	0.43
1:A:223:TRP:O	1:A:230:MET:HA	2.20	0.42
1:A:23:TYR:CD2	1:A:23:TYR:C	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLU:N	1:A:94:PRO:CD	2.83	0.41
1:A:200:ASN:HD22	1:A:200:ASN:N	2.16	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	293/294 (100%)	288 (98%)	5 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	230/253 (91%)	222 (96%)	8 (4%)	36 17

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	9	SER
1	A	51	TRP
1	A	80	PRO

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Mol	Chain	Res	Type
1	A	197	VAL
1	A	200	ASN
1	A	237	SER
1	A	287	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	24	ASN
1	A	86	GLN
1	A	159	GLN
1	A	195	ASN
1	A	200	ASN
1	A	222	GLN
1	A	292	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	295	3,1	42,50,50	1.74	10 (23%)	46,82,82	1.81	11 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	295	3,1	-	3/12/54/54	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	295	HEM	C3C-C2C	-4.61	1.34	1.40
2	A	295	HEM	C3C-C4C	3.25	1.46	1.41
2	A	295	HEM	C3C-CAC	3.00	1.54	1.47
2	A	295	HEM	CAB-C3B	2.86	1.55	1.47
2	A	295	HEM	O2A-CGA	-2.69	1.21	1.30
2	A	295	HEM	C3B-C2B	-2.53	1.32	1.37
2	A	295	HEM	O1A-CGA	2.48	1.30	1.22
2	A	295	HEM	O2D-CGD	-2.45	1.22	1.30
2	A	295	HEM	CMD-C2D	2.29	1.55	1.50
2	A	295	HEM	CHA-C4D	2.09	1.39	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	295	HEM	O2D-CGD-CBD	5.29	130.72	114.00
2	A	295	HEM	C4C-CHD-C1D	4.58	128.60	122.56
2	A	295	HEM	CMC-C2C-C3C	3.77	132.21	124.68
2	A	295	HEM	O2D-CGD-O1D	-3.47	114.42	123.33
2	A	295	HEM	CAA-CBA-CGA	-3.19	105.25	113.83
2	A	295	HEM	O1D-CGD-CBD	-3.01	113.54	123.09
2	A	295	HEM	O2A-CGA-CBA	2.94	123.30	114.00
2	A	295	HEM	CMA-C3A-C4A	-2.57	124.69	128.46
2	A	295	HEM	C4A-C3A-C2A	2.52	108.75	107.00
2	A	295	HEM	C3B-C2B-C1B	2.50	108.28	106.41
2	A	295	HEM	O1A-CGA-CBA	-2.06	116.56	123.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

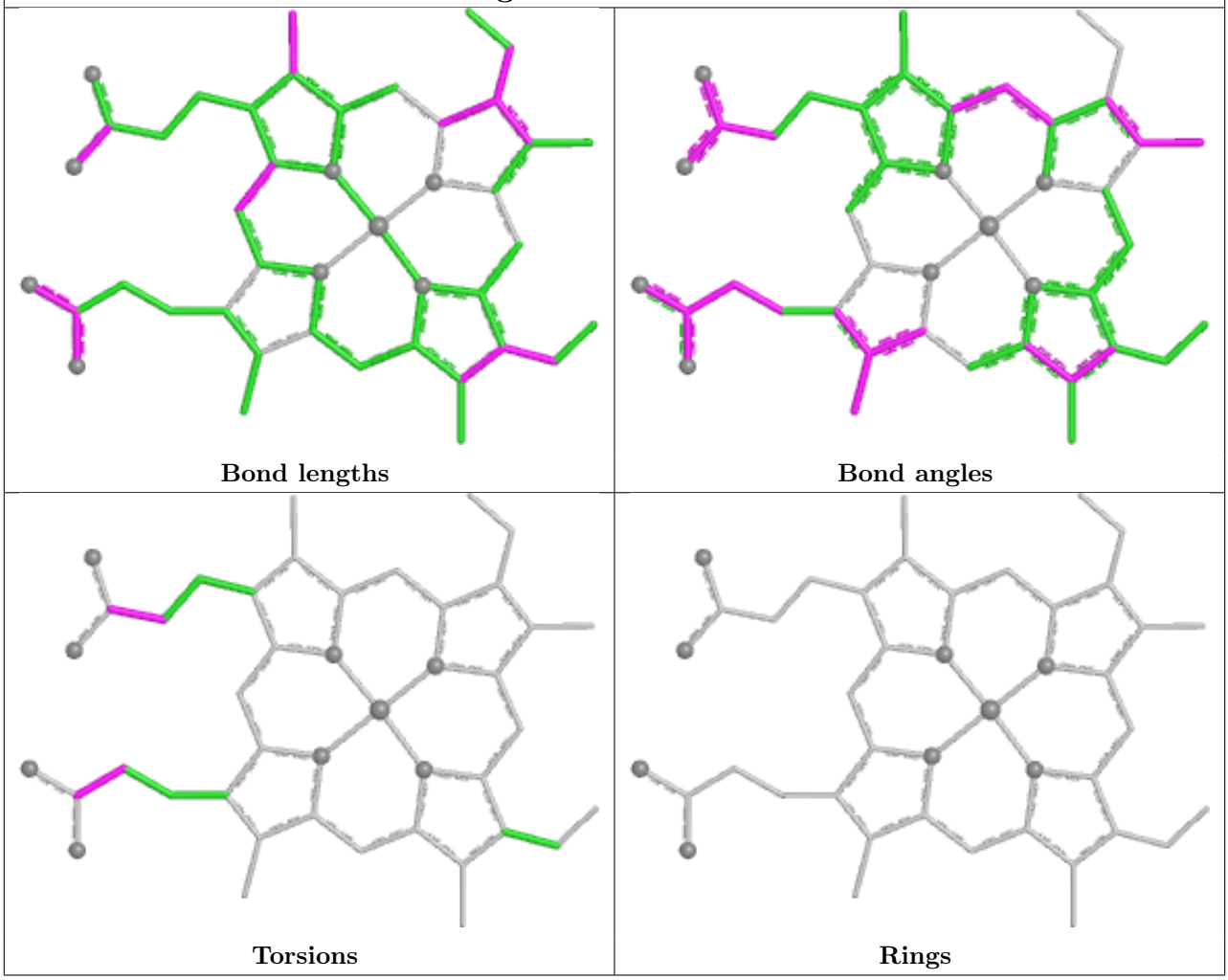
Mol	Chain	Res	Type	Atoms
2	A	295	HEM	CAA-CBA-CGA-O2A
2	A	295	HEM	CAD-CBD-CGD-O1D
2	A	295	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HEM A 295



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	293/294 (99%)	-0.49	3 (1%) 82 85	18, 27, 42, 69	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	THR	5.4
1	A	3	PRO	4.9
1	A	39	TYR	2.5

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

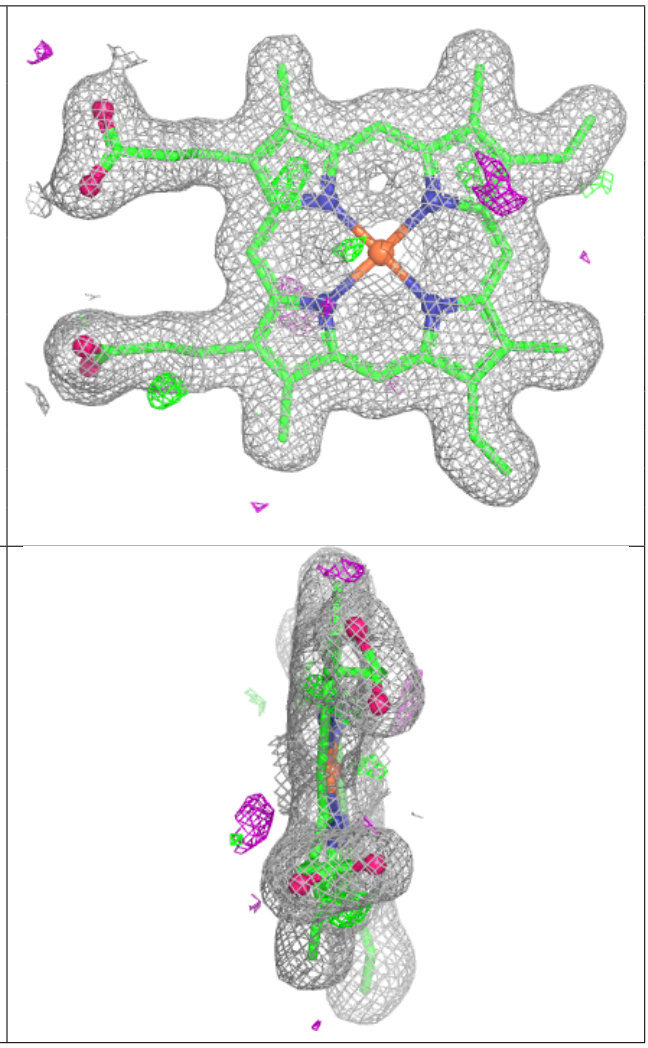
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	O	A	296	1/1	0.90	0.16	34,34,34,34	1
2	HEM	A	295	43/43	0.98	0.06	18,22,25,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEM A 295:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.